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On characteristics of ancestral character-state reconstructions under the accelerated transformation optimization

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Abstract

A combinatorial optimization problem regarding assignments of real numbers (called reconstructions) on a tree has been discussed in phylogenetic analysis. Recently, a clear method for finding most-parsimonious reconstructions (MPRs) on a given end-labeled-tree (phylogenetic tree) has been presented by Hanazawa et at. (Discrete Appl. Math. 56 (1995) 245–265, Narushima and Hanazawa, Discrete Appl. Math. 80 (1997) 231–238). In the framework based on the method, we refine and generalize the accelerated transformation (ACCTRAN) reconstruction which originated with Farris (Syst. Zool. 19 (1970) 92) and was defined more explicitly by Swofford and Maddison (Math. Biosci. 87 (1987) 229). This is considered one of the more meaningful and useful of the possible MPRs. We also generalize the MPR-poset of MPRs, which is introduced by Minaka (Forma 8 (1993) 296). Then two theorems on characteristics of ACCTRANs are given. One shows that the ACCTRAN on a rooted e.l.tree T is the unique MPR on T for which the lengths of all subtrees are minimized, that is, the completeness in most-parsimonious properties of ACCTRANs. Another states some conditions for the ACCTRAN to be the greatest element in the MPR-poset. © 2002 Elsevier Science B.V. All rights reserved.

Keywords: Evolutionary tree; Maximum parsimony; Most-parsimonious reconstraction; Accelerated transformation optimization; MPR-poset

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1. Introduction

Many Biologists have attempted to infer the evolutionary trees whose leaves are present day species. One of the main problems is to assign a character-state to each internal node of a given tree with the leaves to which the character-states of present day species are assigned, so as to minimize the total amount of evolutionary change, and to generate such assignments called most-parsimonious reconstructions (MPRs). In phylogeny, the minimization is also called the maximum parsimony or the Wagner parsimony. The problem and the related problems have been recently called the MPR problems in [3]. The MPR-problems are generally discussed under a given possible transformation relation of character-states. For the problems under a rather general transformation relation, there is a method based on the dynamic programming strategy, which is described in [11]. Especially, under the transformation relation of linearly ordered character-states, Farris [2] and Swofford and Maddison [10] have dealt with the problems on a completely bifurcating phylogenetic tree and given a solution. Hanazawa et al. [3] have mathematically formulated the problems with a generalization to any tree and presented clear algorithms for those, and then evaluated the computational complexity of each of the algorithms. Furthermore, Narushima and Hanazawa [7] have given a more efficient algorithm for one of the MPR problems. On the other hand, noting that generally a phylogenetic tree has more than one MPR, Swofford and Maddison [10] have defined more explicitly the accelerated transformation (ACCTRAN) reconstruction, which originated with [2], and which is considered one of the more meaningful and useful of the possible MPRs. Then Minaka [5] has introduced the usual partial ordering on the set of all possible MPRs on a phylogenetic tree, in order to investigate the relationships between the MPRs.

We here mention two papers which deal with the case of non-tree graphs for the minimization problem, from a purely mathematical point of view independent of phylogenetic analysis. One is the pioneering paper [9]. It shows that for a graph G with vertex set V and a partial real valued function h on V, there exists a total function f on V which is an extension of h and minimizes the sum of $|f(u)-f(v)|$ over all edges $\{u,v\}$ of G, and it derives an algorithm for obtaining such an extension. Another is Hanazawa and Narushima [4] in which a linear algorithm (for the number of vertices) for the case of the unicycle graph is given by applying their previous method. We now have a gap between the Robinson method and the Hanazawa–Narushima one. It is a pose to bridge the gap.

In this paper, in our framework based on the method of Hanazawa and Narushima, we refine and generalize the ACCTRAN reconstruction and the MPR-poset. Then two main theorems on characteristics of ACCTRAN reconstructions are given. One (Theorem 1) shows that the ACCTRAN reconstruction on a rooted tree T is the unique MPR on T for which the lengths of all subtrees are minimized, that is, the completeness in most-parsimonious properties of the ACCTRAN reconstruction. Another (Theorem 2) states some conditions for the ACCTRAN reconstruction to be the greatest element in the MPR-poset. An introductory part of this paper is shown in [8].

We use the notations in [3,7]. Let Ω denote the set that may be either the set $\mathbf{R}$ of real numbers or the set $\mathbf{N}$ of nonnegative integers. Note that Ω expresses the linearly

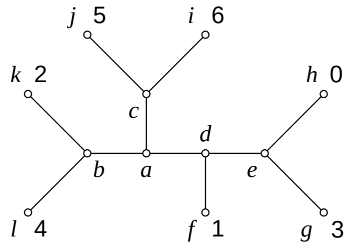


Fig. 1. An e.l.tree T.

Table 1
The set $\mathrm{Rmp}(T)$ of all MPRs

$\lambda \backslash u$	a	b	c	d	e	f	g	h	i	j	k	l
λ_1	2	2	5	1	1	1	3	0	6	5	2	4
λ_2	2	2	5	2	2	1	3	0	6	5	2	4
λ_3	3	3	5	1	1	1	3	0	6	5	2	4
λ_4	3	3	5	2	2	1	3	0	6	5	2	4
λ_5	3	3	5	3	3	1	3	0	6	5	2	4
λ_6	4	4	5	1	1	1	3	0	6	5	2	4
λ_7	4	4	5	2	2	1	3	0	6	5	2	4
λ_8	4	4	5	3	3	1	3	0	6	5	2	4

ordered character-states. Let $T=(V=V_O \cup V_H, E, \sigma)$ be any undirected tree with the endnodes evaluated by a weight function $\sigma: V_O \to \Omega$, where V is the set of nodes, V_O is the set of endnodes, V_H is the set of internal nodes, and E is the set of branches. This tree is called an end-labeled-tree (e.l.tree). An e.l.tree T is shown in Fig. 1. Note that the examples are shown in Section 4. For an e.l.tree T, we define an assignment $\lambda: V \to \Omega$ such that $\lambda \mid V_O$ (the restriction of λ to V_O) $=\sigma$, where $\lambda(v)$ is called a *state* of v under λ. This assignment is called a *reconstruction* on an e.l.tree T. For each branch e in E of an e.l.tree T with a reconstruction λ, we define the *length* $l(e)$ of branch $e=\{u,v\}$ by $|\lambda(u)-\lambda(v)|$. Then the *length* $L(T,\lambda)$ of an e.l.tree T under the reconstruction λ is the sum of the lengths of the branches. That is $L(T,\lambda)=\sum_{e\in E} l(e)$. Furthermore, we define the minimum length $L^*(T)$ of T by

$$L^*(T)=\min\{L(T,\lambda) \mid \lambda \text{ is a reconstruction on } T\}.$$

Note that $L^*(T)$ is well-defined. A MPR on an e.l.tree T is a reconstruction λ such that $L(T,\lambda)=L^*(T)$. Generally an e.l.tree T has more than one MPR. All MPRs on T in Fig. 1 are shown in Table 1, where $L^*(T)=10$. The set $\{\lambda(u) \mid \lambda \text{ is an MPR on } T\}$ of states is called the MPR-*set* of a node u and written as S_u. For example, we see from Table 1 that $S_a=S_b=[2,4]$, $S_c=[5,5]$ and $S_d=S_e=[1,3]$.

The main MPR problems are described as follows: for a given e.l.tree T, 1: determine $L^*(T)$, 2: find any one MPR on T, 3: enumerate all MPRs on T, and 4: obtain the MPR-sets for all internal nodes in T. For their meanings in phylogeny, the reader may refer to [10,11]. As previously stated, the problems on a completely bifurcating phylogenetic tree have been solved in [2,10], and then a clear method for solving the problems on any tree has been presented in [3,7]. A more efficient algorithm for the MPR problems than one in [3] is given in [7]. That is, the complexity of the algorithm in [3] for Problem 4 is $O(n^2)$ for the number n of nodes in a given e.l.tree, but that of the algorithm in [7] is $O(n)$. Note that the number of comparisons required to select the ith smallest of n numbers is essential in the complexity analysis of the algorithm, and therefore the time complexity analysis is based on the complexity of the selection algorithm called PICK by Blum et al. [1]. The theorem in [7], on which the linear algorithm for Problem 4 is based, plays an important role in this paper.

2. Preliminaries

We begin by reviewing the key concepts and results in the previous papers [3,7] which are used in this paper. Let $a_1,\dots,a_{2n}$ be any elements in Ω, and be sorted in ascending order as follows:

$$x_1 \leqslant \cdots \leqslant x_n \leqslant x_{n+1} \leqslant \cdots \leqslant x_{2n}.$$

Then we call x_n and x_{n+1} the *median two points* of the numbers $a_1,\dots,a_{2n}$, and denote the sequence $\langle x_n, x_{n+1}\rangle$ by

$$\mathrm{med2}\langle a_1,\dots,a_{2n}\rangle.$$

We also call $x_{n-1},\ x_n,\ x_{n+1}$ and x_{n+2} the *median four points* of the numbers $a_1,\dots,a_{2n}$, and denote the sequence $\langle x_{n-1},x_n,x_{n+1},x_{n+2}\rangle$ by

$$\mathrm{med4}\langle a_1,\dots,a_{2n}\rangle.$$

The following is Lemma 1 in [7], which is frequently used in this paper.

Lemma A. *Let a any element in Ω. Let $b_1,\dots,b_{2n}$ be any elements in Ω, of which median four points are c_1,c_2,c_3,c_4. Then*

$$\mathrm{med2}\langle a,a,b_1,\dots,b_{2n}\rangle = \mathrm{med2}\langle a,a,c_1,c_2,c_3,c_4\rangle.$$

Let $I_1=[a_1,b_1],\dots,I_m=[a_m,b_m]$ be any family of closed intervals in Ω. Then we denote the ordered pair $\mathrm{med2}\langle a_1,\dots,a_m,b_1,\dots,b_m\rangle$ by

$$\mathrm{med2}\langle I_1,\dots,I_m\rangle.$$

We also denote the quadruple $\mathrm{med4}\langle a_1,\dots,a_m,b_1,\dots,b_m\rangle$ by

$$\mathrm{med4}\langle I_1,\dots,I_m\rangle.$$

Let $\mathrm{med2}\langle I_1,\dots,I_m\rangle=\langle x_m,x_{m+1}\rangle$. Then we call the closed interval $[x_m,x_{m+1}]$ in Ω the *median interval* of the closed intervals $I_1,\dots,I_m$, which is the key concept in a series of our papers, and denote it by

$$\mathrm{med}\langle I_1,\dots,I_m\rangle \quad \text{or} \quad \mathrm{med}\langle I_i\colon i=1,\dots,m\rangle.$$

Let $T=(V,E)$ be a rooted (directed) tree, where V is the set of nodes and E ($\subseteq V\times V$) is the set of branches. For each u and v in V, we write $u=p(v)$ when $(u,v)\in E$, that is, when u is a *parent* of v (or v is a *child* of u). This relation $(p(v), v)$ on V is called a *parent–child relation*. For each u and v in V, u is called an *ancestor* of v (or v is called a *descendent* of u), if there is a sequence of nodes $u = u_1, u_2, \ldots, u_n = v$ in V such that $u_i = p(u_{i+1})$ $(i = 1, \ldots, n-1)$. In a rooted tree, there is only one node without a parent, which is called the *root*, and a node without a child is called a *leaf*. For each u in V, we denote a *subtree* of T induced from a subset $\{u\} \cup \{v \in V \mid v$ is a descendant of $u\}$ of V by $T_u = (V_u, E_u)$. Note that u is the root of T_u.

An e.l.tree $T = (V_O \cup V_H, E, \sigma)$ and an element r of $V = V_O \cup V_H$ give rise to a unique directed e.l.tree rooted by r, which is denoted by $T^{(r)}$. The rooted e.l.tree $T^{(r)}$ is simply written T if it is understood. In addition, if r is an endnode, i.e., $r \in V_O$ and s is its unique child, we denote the rooted tree $T^{(r)}$ by (T_s, r) to visualize the structure. In this case, the subtree T_s is called the *body* of the tree $T^{(r)}$; otherwise, i.e., if $r \in V_H$, the body of $T^{(r)}$ is $T^{(r)}$ itself. An rooted e.l.tree $T^{(f)} = (T_d, f)$ is shown in Fig. 3(a).

For each node u in the body of a rooted e.l.tree T, we assign a closed interval $I(u)$ of Ω recursively as follows:

$$I(u) = \begin{cases} [\sigma(u), \sigma(u)] & \text{if } u \text{ is a leaf,} \\ \mathrm{med}\langle I(v)\colon v \text{ is a child of} u\rangle & \text{otherwise.} \end{cases}$$

We call $I(u)$ the *characteristic interval* of a node u and so I is called the *characteristic interval map* on T. The map I is considered to be a fine generalization of the Farris interval in [10]. Let T be a rooted e.l.tree (T_s, r) and I be the characteristic interval map on T. Let $\lambda_{\langle u\rangle}$ denote the restriction $\lambda \mid (T_u, p(u))$ of a reconstruction λ on T. We define a set $\mathrm{Rmp2}(r, s)$ of reconstructions on $T = (T_s, r)$ recursively as follows:

$$\lambda_{\langle s\rangle} \in \mathrm{Rmp2}(r,s) \quad \Leftrightarrow \quad \begin{cases} \lambda(s) \in \mathrm{med}\langle[\lambda(r), \lambda(r)], I(t_1), \ldots, I(t_n)\rangle, & \text{and} \\ \lambda_{\langle t_i\rangle} \in \mathrm{Rmp2}(s, t_i),\ i = 1, \ldots, n & \end{cases}$$

where $t_1, \ldots, t_n$ be the children of s. Note that

$$\lambda_{\langle s\rangle} = \lambda|(T_s, p(s)) = \lambda|(T_s, r) = \lambda$$

can be considered a reconstruction on T. The following is Theorem 1 (Theorem 3(ii)) in [3] (Fig. 2).

Theorem B. *For any endnode r of an e.l.tree T,* $\mathrm{Rmp2}(r,s)$ *is the set of all* MPRs *on T.*

The set of all MPRs on $T^{(f)}$ of Fig. 3(a) is shown in Table 1. From Theorem B, we see that if $v_1, \ldots, v_n$ be the children of u, the interval

$$\mathrm{med}\langle [x,x], I(v_1), \ldots, I(v_n)\rangle$$

is the MPR-set of node u w.r.t. the rooted e.l.tree $(T_u, p(u))$ with $p(u)$ labeled with x. If x is in $S_{p(u)}$, this interval is a subset of S_u and s denoted by $S_u \mid x$. Since it is a key concept in dealing with the MPR problems, we often use it in our discussion and it figures in many of our results. The following is Theorem 1 in [7], which plays an important role in this paper.

Theorem C. *Let T be a rooted e.l.tree (T_s, r). Then each* MPR-*set S_u for each internal node u of T is recursively determined by*

$$S_u = [\min(S_u \mid \min(S_{p(u)})), \max(S_u \mid \max(S_{p(u)}))].$$

The MPR-sets S_u for internal nodes u of $T^{(f)}$ of Fig. 3(a) are shown in Fig. 3(b).

3. The main theorems

We now state the main concepts and results in this paper. First of all, we refine and generalize the ACCTRAN reconstruction on any rooted tree, which was defined on a rooted tree (T_s, r) with a binary tree T_s in [10]. The ACCTRAN accelerates changes (transformations) as soon as possible with respect to the specified root r, hence its name. The mathematical base is later on shown in the Corollary 1. A biological implication is that ACCTRAN maximizes *reversals*, but that is beyond the scope of this paper. For details see [2,5,10,11]. We here examine rather the mathematical aspects of the reconstruction. The ACCTRAN algorithm introduced in [10] for binary trees is easily refined and generalized by using the related results in [3,7].

Let a, b and c be any elements in Ω. Then we denote the median point of a, b and c by median$\langle a, b, c\rangle$. Let I be the characteristic map on a rooted e.l.tree $T = (T_s, r)$. Then we define a reconstruction λ_{ACT} on T recursively from the root r to leaves as follows: $\lambda_{\mathrm{ACT}}(r) = \sigma(r)$ and for each internal node u,

$$\lambda_{\mathrm{ACT}}(u) = \mathrm{median}\langle \lambda_{\mathrm{ACT}}(p(u)), \min(I(u)), \max(I(u))\rangle.$$

Note that $\min(I(u))$ is the left endpoint of the closed interval $I(u)$ and $\max(I(u))$ is the right endpoint of the closed interval $I(u)$. It is immediate from the definitions that λ_{ACT} is the ACCTRAN reconstruction on T defined by Swofford and Maddison [10] when T_s is binary. So we call λ_{ACT} the ACCTRAN reconstruction on T. The ACCTRAN reconstruction λ_{ACT} on $T^{(f)}$ of Fig. 3(a) is shown in Fig. 3(b). We now have the following results which lead to the main theorems in this paper.

Lemma 1 (The median map lemma). *Let x be any element in Ω. Let a, b, c and d be any elements in Ω such that $a \leqslant b \leqslant c \leqslant d$. Then,*

$$(1)\ \mathrm{median}\langle x, b, c\rangle = \begin{cases} b & (x \leqslant b), \\ x & (b \leqslant x \leqslant c), \\ c & (c \leqslant x). \end{cases}$$

$$(2)\ \mathrm{med2}\langle x, x, a, b, c, d\rangle = \begin{cases} \langle a, b\rangle & (x \leqslant a), \\ \langle x, b\rangle & (a \leqslant x \leqslant b), \\ \langle x, x\rangle & (b \leqslant x \leqslant c), \\ \langle c, x\rangle & (c \leqslant x \leqslant d), \\ \langle c, d\rangle & (d \leqslant x). \end{cases}$$

Proof. By the definition. □

Proposition 1. *Let T be a rooted e.l.tree (T_s, r). Let λ be the* ACCTRAN *reconstruction λ_{ACT} on T. Then for any internal node u of T, $\lambda(u)$ is equal to the element in $I(u)$ closest to $\lambda(p(u))$.*

Proof. Obvious. □

Lemma 2. *Let x be any element in Ω. Let $I_1, \ldots, I_n$ be any closed intervals in Ω. Let* $\mathrm{med2}\langle I_1, \ldots, I_n\rangle = \langle a, b\rangle$. *Then*

$$\mathrm{median}\langle x, a, b\rangle \in \mathrm{med}\langle [x,x], I_1, \ldots, I_n\rangle.$$

Proof. Obvious. □

Proposition 2. *The* ACCTRAN *reconstruction λ_{ACT} on a rooted e.l.tree $T = (T_s, r)$ is an* MPR *on T.*

Proof. We see from Theorem B that it is sufficient to show the following: for each internal node u of T, $\lambda_{\mathrm{ACT}}(u) \in S_u \mid \lambda_{\mathrm{ACT}}(p(u))$ when $\lambda_{\mathrm{ACT}}(p(u)) \in S_{p(u)}$. We first note that from the definition of a reconstruction, $p(s) = r$ and S_r is a singleton $\{\lambda_{\mathrm{ACT}}(r) = \sigma(r)\}$. Then, considering the definitions of $\lambda_{\mathrm{ACT}}(u)$, $S_u \mid \lambda_{\mathrm{ACT}}(p(u))$, and

$$\mathrm{med2}\langle I(v)\text{: } v \text{ is a child of } u\rangle = \langle \min(I(u)), \max(I(u))\rangle$$

from the definition of the characteristic interval I, we can show the proposition by applying Lemma 2 to this case with

$$x = \lambda_{\mathrm{ACT}}(p(u)) \quad \text{and} \quad \langle I_1, \ldots, I_m\rangle = \langle I(v)\text{: } v \text{ is a child of } u\rangle. \qquad \square$$

Lemma 3 (The singleton lemma). *Let x be any element in Ω. Let $I_1, \ldots, I_n$ be any closed intervals in Ω. Then* $\mathrm{med}\langle I_1, \ldots, I_n\rangle \cap \mathrm{med}\langle [x,x], I_1, \ldots, I_n\rangle$ *is a singleton.*

Proof. Obvious. □

Proposition 3. *Let T be a rooted e.l.tree (T_s, r). Then for any internal node u of T and any element x in $S_{p(u)}$, $S_u \mid x \cap I(u)$ is a singleton.*

Proof. Since

$$S_u \mid x = \mathrm{med}\langle [x,x], I(v_1), \ldots, I(v_n)\rangle \quad \text{and} \quad I(u) = \mathrm{med}\langle I(v_1), \ldots, I(v_n)\rangle,$$

where $v_1, \ldots, v_n$ be the children of u, by Lemma 3 the proof is complete. □

The following is Corollary 4 in [3].

Corollary D. *Let T be a rooted e.l.tree (T_s, r), and u an internal node of T. Then for any x, there is an* MPR *λ for a subtree T_u such that $\lambda(u) = x$, if and only if $x \in I(u)$.*

Proposition 4. *Let T be a rooted e.l.tree (T_s, r). Then there is only one reconstruction λ on T such that $L(T_u, \lambda_{\langle u\rangle}) = L^*(T_u)$ for all u in V, where $\lambda_{\langle u\rangle}$ denotes the restriction of λ to a subtree T_u of T.*

Proof. By Proposition 3, we can well define an MPR λ on T recursively by

$$\lambda(u) = \text{the unique element of } S_u \mid \lambda(p(u)) \cap I(u).$$

Theorem B asserts that this λ is an MPR. The uniqueness follows from Corollary D. □

The reconstruction λ in Proposition 4 is quite remarkable for its property. So, we call the property *the complete maximum-parsimonity*. We are now ready to describe the first main theorem in this paper.

Theorem 1. *The* ACCTRAN *reconstruction λ on a rooted e.l.tree $T = (T_s, r)$ is the* MPR *with the complete maximum-parsimonity, that is, λ is the unique* MPR *on T for which the lengths of all the subtrees are minimized.*

Proof. For any internal node u of T, $\lambda(u) \in I(u)$ by Proposition 1 and $\lambda(u) \in S_u \mid \lambda(p(u))$ by Proposition 2. Therefore, we have

$$\lambda(u) \in (S_u \mid \lambda(p(u)) \cap I(u)).$$

Thus, by the definition of the MPR with the complete maximum-parsimonity we complete the proof. □

An example illustrating Theorem 1 is shown in Fig. 3(c). From Theorem 1, we now get the following generalization of the statement implicitly described for the binary case in [10, p. 222].

Corollary 1. *Let λ be the* ACCTRAN *reconstruction on a rooted e.l.tree $T = (T_s, r)$ and u be any internal node in T. Let μ be any* MPR *on T such that $\mu(p(u)) = \lambda(p(u))$. Then*

$$|\lambda(p(u)) - \lambda(u)| \geqslant |\mu(p(u)) - \mu(u)|.$$

Proof. The restriction $\lambda \mid (T_u, p(u))$ of λ is considered to be an MPR on the rooted e.l.tree $(T_u, p(u))$ with $\sigma(p(u)) = \mu(p(u)) = \lambda(p(u))$ and so is $\mu \mid (T_u, p(u))$. Therefore by Theorem B, for the rooted e.l.tree $(T_u, p(u))$ we have

$$\begin{aligned} L^*((T_u, p(u))) &= |\lambda(p(u)) - \lambda(u)| + L(T_u, \lambda_{\langle u\rangle}) \\ &= |\mu(p(u)) - \mu(u)| + L(T_u, \mu_{\langle u\rangle}). \end{aligned}$$

Then

$$|\lambda(p(u)) - \lambda(u)| - |\mu(p(u)) - \mu(u)| = L(T_u, \mu_{\langle u\rangle}) - L(T_u, \lambda_{\langle u\rangle}).$$

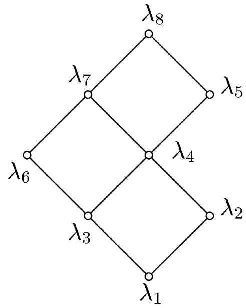


Fig. 2. The MPR-poset (Rmp(T), $\leqslant$).

From Theorem 1, we have

$$L(T_u, \mu_{\langle u\rangle}) - L(T_u, \lambda_{\langle u\rangle}) = L(T_u, \mu_{\langle u\rangle}) - L^*(T_u) \geqslant 0,$$

completing the proof. □

Corollary 1 shows that from the root to the leaves, the ACCTRAN reconstruction on a rooted e.l.tree $T = (T_s, r)$ always assigns the maximum possible amount of change to each branch, given the state assignments made so far. This fact is the base of the name *accelerated transformation optimization* (ACCTRAN). The property of the ACCTRAN reconstruction is reflected in reversals of earlier changes in the same lineage than in parallel changes in different lineages (see [10]).

We next describe the second key concept in this paper. The set of all MPRs on an e.l.tree T is denoted by Rmp(T). Minaka [5,6] introduces the usual partial ordering on Rmp(T) in order to investigate the relationships between the MPRs. For any λ and μ in Rmp(T), the partial ordering $\lambda \leqslant \mu$ is defined by $\lambda(u) \leqslant \mu(u)$ for all u in V. We call the partially ordered set (Rmp(T), $\leqslant$) the MPR-poset or Minaka poset. The MPR-poset (Rmp(T), $\leqslant$) for an e.l.tree T of Fig. 1 is shown in Fig. 2. Note that in the examples in this paper, Ω is restricted to the set $\mathbf{N}$ of nonnegative integers. We first answer whether there exists a unique greatest element (or a unique least element) in the MPR-poset or not.

Lemma 4. *Let λ be a reconstruction on an e.l.tree T defined by*

$$\lambda(u) = \max(S_u)$$

for each internal node u. Let T be rooted at an endnode r and then $T = (T_s, r)$. Let μ be a reconstruction on (T_s, r) defined recursively by

$$\mu(u) = \max(S_u \mid \mu(p(u)))$$

for each internal node u. Then $\lambda = \mu$.

(*The dual case also holds*: *one by replacing* max *with* min.)

Proof. We first prove the equality by induction on the nodes with the parent-child relation. Since $S_s \mid \mu(p(s)) = S_s$, we have $\mu(s) = \lambda(s)$. Assume that $\mu(p(u)) = \lambda(p(u))$ for an internal node u. Then

$$\mu(u) = \max(S_u \mid \mu(p(u))),$$

(by $\mu(p(u)) = \max(S_{p(u)})$ from the assumption)

$$= \max(S_u \mid \max(S_{p(u)})),$$

(by Theorem C)

$$= \max(S_u) = \lambda(u).$$

One can similarly prove the dual case. □

Let $\lambda_{\max}$ denote a reconstruction λ on an e.l.tree T such that $\lambda(u) = \max(S_u)$ for any internal node u. Let $\lambda_{\min}$ denote a reconstruction λ on an e.l.tree T such that $\lambda(u) = \min(S_u)$ for any internal node u. Then, we get the following answer to the preceding question.

Proposition 5. *Let T be an e.l.tree. Then the reconstruction $\lambda_{\max}$ on T is the greatest element of the* MPR-*poset* $(\mathrm{Rmp}(T), \leqslant)$ *and the reconstruction $\lambda_{\min}$ on T is the least element of the* MPR-*poset* $(\mathrm{Rmp}(T), \leqslant)$.

Proof. Obvious by Lemma 4. □

Proposition 6. *Let λ be the* ACCTRAN *reconstruction on a rooted e.l.tree $T = (T_s, r)$. Let u be any internal node of T. Then,*
(1) $\lambda(p(u)) < \lambda(u)$ *if and only if* $\lambda(p(u)) < \min(I(u))$,
(2) $\lambda(p(u)) = \lambda(u)$ *if and only if* $\lambda(p(u)) \in I(u)$,
(3) $\lambda(p(u)) > \lambda(u)$ *if and only if* $\lambda(p(u)) > \max(I(u))$.

Proof. Trivial by the definition of ACCTRAN reconstruction. □

Proposition 7. *Let λ be the* ACCTRAN *reconstruction on a rooted e.l.tree $T = (T_s, r)$. Then for any internal node u, $\lambda(p(u)) \leqslant \lambda(u)$ if and only if $\lambda(p(u)) \leqslant \max(I(u))$.*

(*The dual case also holds: one by replacing* $\leqslant$ *and* max *with* $\geqslant$ *and* min, *respectively.*)

Proof. Obvious by Proposition 6. □

Lemma 5. *Let x be any element in Ω. Let a, b, c and d be any elements in Ω such that $a \leqslant b \leqslant c \leqslant d$.*
(1) *If $x \leqslant c$ then* $\mathrm{median}\langle x, b, c\rangle = \max(\mathrm{med2}\langle x, x, a, b, c, d\rangle)$.
(2) *If $x \geqslant b$ then* $\mathrm{median}\langle x, b, c\rangle = \min(\mathrm{med2}\langle x, x, a, b, c, d\rangle)$.

(3) *Let* $c < d$. *If* $\mathrm{median}\langle x,b,c\rangle = \max(\mathrm{med2}\langle x,x,a,b,c,d\rangle)$ *then* $x \leqslant c$.
(4) *Let* $a < b$. *If* $\mathrm{median}\langle x,b,c\rangle = \min(\mathrm{med2}\langle x,x,a,b,c,d\rangle)$ *then* $x \geqslant b$.

Proof. Trivial. □

Proposition 8. *Let* λ *be the* ACCTRAN *reconstruction on a rooted e.l.tree* $T=(T_s,r)$. *Let* u *be any internal node. Then,*
(1) *if* $\lambda(p(u)) \leqslant \lambda(u)$, *then* $\lambda(u) = \max(S_u \mid \lambda(p(u)))$,
(2) *if* $\lambda(p(u)) \geqslant \lambda(u)$, *then* $\lambda(u) = \min(S_u \mid \lambda(p(u)))$.
Suppose additionally, $\langle a,b,c,d\rangle = \mathrm{med4}\langle I(v)$: v *is a child of* $u\rangle$. *Then*:
(3) *If* $c < d$ *and* $\lambda(u) = \max(S_u \mid \lambda(p(u)))$ *then* $\lambda(p(u)) \leqslant \lambda(u)$.
(4) *If* $a < b$ *and* $\lambda(u) = \min(S_u \mid \lambda(p(u)))$ *then* $\lambda(p(u)) \geqslant \lambda(u)$.
(5) *If* $c < d$, *then* $\lambda(p(u)) \leqslant \lambda(u)$ *if and only if* $\lambda(u) = \max(S_u \mid \lambda(p(u)))$.
(6) *If* $a < b$, *then* $\lambda(p(u)) \geqslant \lambda(u)$ *if and only if* $\lambda(u) = \min(S_u \mid \lambda(p(u)))$.

Proof. Suppose that λ is ACCTRAN, u is an internal node, $\langle a,b,c,d\rangle = \mathrm{med4}\langle I(v)$: v is a child of $u\rangle$. Then, (1) and (2) are immediate from Proposition 7 and Lemma 5(1) and (2). (3) and (4) are from Proposition 7 and Lemma 5(3) and (4). (5) and (6) are from (1–4). More directly, we see the following by the definitions of the notations $S_u \mid x$ and ACCTRAN. Let $x = \lambda(p(u))$. Then,
(a) if $x \leqslant b$, then $S_u \mid x = [\max(a,x), b]$ and $\lambda(u) = b$,
(b) if $b \leqslant x \leqslant c$, then $S_u \mid x = \{x\}$ and $\lambda(u) = x$,
(c) if $c \leqslant x$, then $S_u \mid x = [c, \min(x,d)]$ and $\lambda(u) = c$.
Obviously this shows the proposition. □

Let $T = (T_s, r)$ be a rooted e.l.tree. Let λ be a reconstruction on T such that $\lambda(p(u)) \leqslant \lambda(u)$ for any internal node u. Then λ is said to be *monotone increasing on the Ancestral domain* (*A.-domain*). It means phylogenetically that each ancestral character-state under the reconstruction λ is monotonically increasing from the root to the most recent ancestors. Also, a *monotone decreasing reconstruction on the A.-domain* is dually defined. We are now ready to describe the second main theorem in this paper.

Theorem 2. *Let* λ *be the* ACCTRAN *reconstruction on a rooted e.l.tree* $T = (T_s, r)$.
(1) *If* λ *is monotone increasing on the A.-domain*, *then* λ *is the greatest element* $\lambda_{\max}$ *of the* MPR-*poset* $(\mathrm{Rmp}(T), \leqslant)$.
(2) *Let the third element of* $\mathrm{med4}\langle I(v) : u \to v\rangle$ *be strictly less than the fourth element of* $\mathrm{med4}\langle I(v) : u \to v\rangle$ *for all internal nodes u. If* λ *is the greatest element* $\lambda_{\max}$ *of the* MPR-*poset* $(\mathrm{Rmp}(T), \leqslant)$, *then* λ *is monotone increasing on the A.-domain.*

(*The dual case also holds*: *one by replacing* increasing, greatest, $\lambda_{\max}$, third *and* fourth *with* decreasing, least, $\lambda_{\min}$, first *and* second, *respectively*.)

Proof. By induction on the internal nodes with the parent–child relation, the proof is immediate from the preceding results. (1) follows from Proposition 8(1) and (2), Lemma 4 and Proposition 5. (2) follows from Proposition 8(3) and (4), Lemma 4 and Proposition 5. □

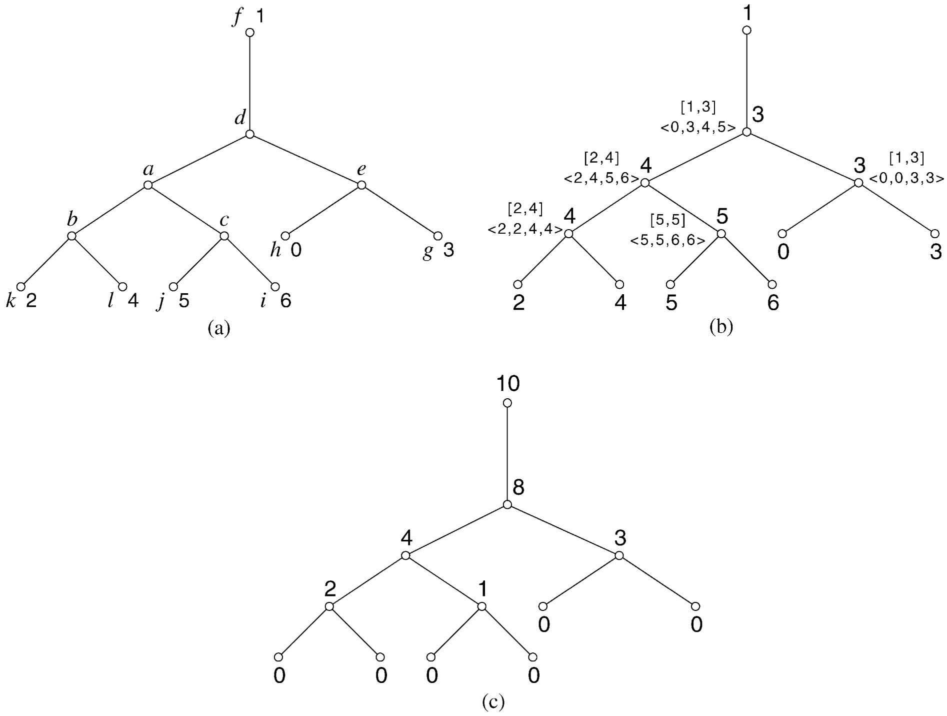


Fig. 3. Example 1 of Theorems 1 and 2(1).

Corollary 2. *Let* λ *be the* ACCTRAN *reconstruction on a rooted e.l.tree* $T=(T_s,r)$. *Let the third element of* $\text{med4}\langle I(v):u\to v\rangle$ *be strictly less than the fourth element of* $\text{med4}\langle I(v):u\to v\rangle$ *for any internal node u. Then,* λ *is monotone increasing on the A.-domain if and only if* λ *is the greatest element* $\lambda_{\max}$ *of the* MPR-*poset* $(\text{Rmp}(T),\leqslant)$.

(*The dual case also holds*: *one by replacing* third, fourth, increasing, greatest *and* $\lambda_{\max}$ *with* first, second, decreasing, least *and* $\lambda_{\min}$, *respectively*.)

Proof. It is immediate from Theorem 2 (or Proposition 8(5) and (6)). $\square$

4. Examples

We here show some examples for illustrating the preceding results. In the examples, Ω is restricted to the set $\mathbf{N}$ of nonnegative integers. An e.l.tree T hereafter used, is shown in Fig. 1, which is also given in [3]. Note that

$$\sigma(f)=1,\quad \sigma(g)=3,\quad \sigma(h)=0,\quad \sigma(i)=6,\quad \sigma(j)=5,\quad \sigma(k)=2,\quad \sigma(l)=4.$$

All MPRs on T are recursively generated by the algorithm of Hanazawa and Narushima and shown in Table 1 (also given in [3]). Then we have the MPR-poset $(\text{Rmp}(T),\leqslant)$

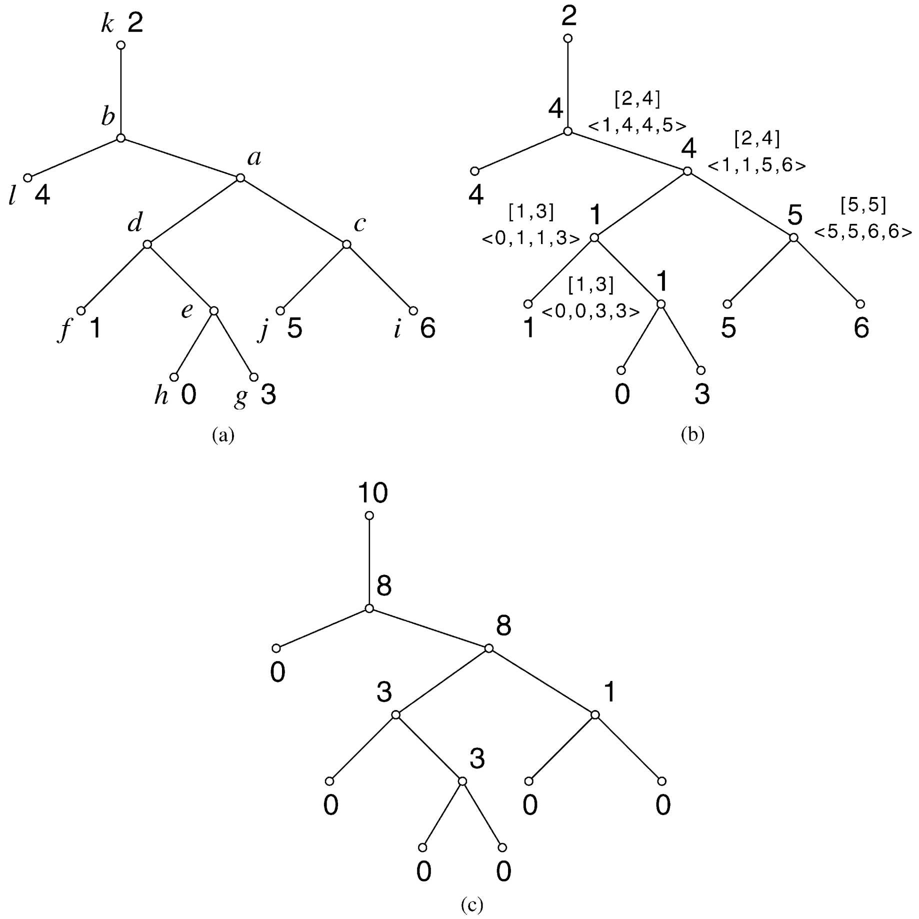
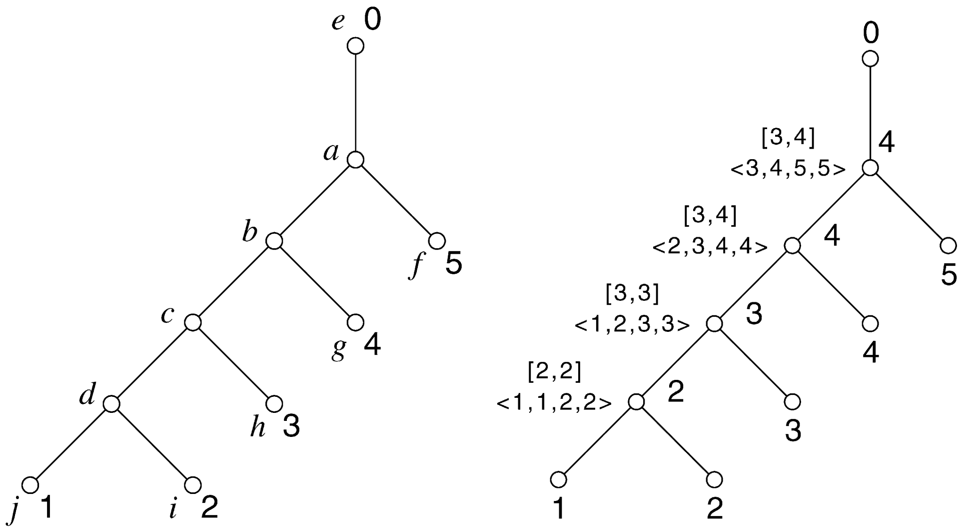


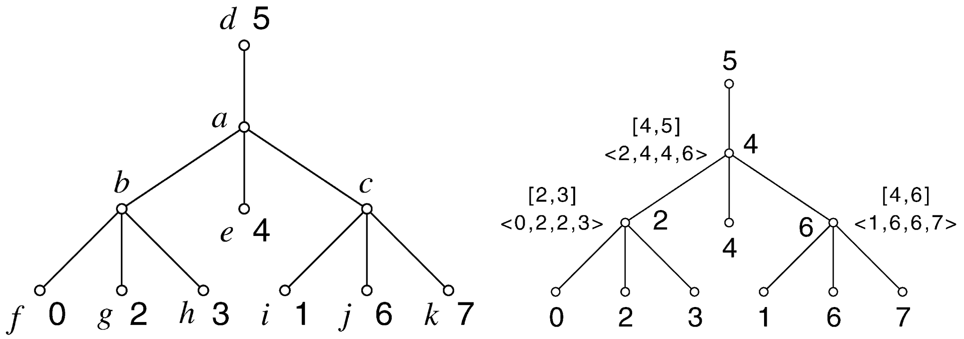
Fig. 4. Example 2 of Theorems 1 and 2(1).

shown in Fig. 2. Let the e.l.tree T in Fig. 1 be rooted at f. Then we have a rooted e.l.tree $T^{(f)} = (T_d, f)$ shown in Fig. 3(a), and the ACCTRAN reconstruction λ_{ACT} on $T^{(f)}$ shown in Fig. 3(b), with med4$\langle I(v)$: v is a child of $u\rangle$ and MPR-set S_u for each internal node u. In Fig. 3(c), the value of each node u represents the minimum length $L^*(T_u)$ of each subtree T_u, which illustrates Theorem 1. Furthermore, note that the λ_{ACT} is monotone increasing on the A.-domain and then the λ_{ACT} is equal to λ_8, the greatest element $\lambda_{\max}$ of the MPR-poset shown in Fig. 2. This fact shows that it is an example of Theorem 2(1). Let the e.l.tree T in Fig. 1 be rooted at k. Then we have another rooted e.l.tree $T^{(k)} = (T_b, k)$ shown in Fig. 4(a), and the ACCTRAN reconstruction λ_{ACT} on $T^{(k)}$ shown in Fig. 4(b). In Fig. 4(c), the value of each node u represents the minimum length $L^*(T_u)$ of each subtree T_u, which illustrates Theorem 1. Furthermore, note that the λ_{ACT} is not monotone increasing on the A.-domain and then



(a) (b)

Fig. 5. A counterexample for the converse of Theorem 2(1).



(a) (b)

Fig. 6. An example satisfying the additional condition.

the λ_{ACT} is equal to λ_6 which is not the greatest element of the MPR-poset shown in Fig. 2. This example shows the necessity of the monotonicity condition on λ to be the greatest element. But it is shown in the following example that the necessity does not necessarily hold. The ACCTRAN reconstruction on a rooted e.l.tree $T^{(e)} = (T_a, e)$ given in Fig. 5 is the greatest element of the MPR-poset, but not monotone increasing on the A.-domain. This fact shows that the converse of Theorem 2(1) does not necessarily hold. The last example shown in Fig. 6 is one satisfying the additional condition: for each internal node u, the third (first) element of $\mathrm{med4}\langle I(v)\colon v \text{ is a child of } u\rangle$ is strictly less than the fourth (second) element of $\mathrm{med4}\langle I(v)\colon v \text{ is a child of } u\rangle$.

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References

[1] M. Blum, R.W. Floyd, V. Pratt, R.L. Rivest, R.E. Tarjan, Time bounds for selection, J. Comput. System Sci. 7 (1973) 448–461.
[2] J.M. Farris, Methods for computing Wagner trees, Syst. Zool. 19 (1970) 83–92.
[3] M. Hanazawa, H. Narushima, N. Minaka, Generating most parsimonious reconstructions on a tree: a generalization of the Farris–Swofford–Maddison method, Discrete Appl. Math. 56 (1995) 245–265.
[4] M. Hanazawa, H. Narushima, The lightest totalization of an endnode labelling of a non-tree graph II, Proc. Schl. Sci. Tokai Univ. 35 (2000) 7–19.
[5] N. Minaka, Parsimony, phylogeny and discrete mathematics: combinatorial problems in phylogenetic systematics, Natural History Research, Chiba Prefectural Museum and Institute, Vol. 2, No. 2, 1993, pp. 83–98 (in Japanese: with English summary).
[6] N. Minaka, Algebraic properties of the most parsimonious reconstructions of the hypothetical ancestors on a given tree, Forma 8 (1993) 277–296.
[7] H. Narushima, M. Hanazawa, A more efficient algorithm for MPR problems in phylogeny, Discrete Appl. Math. 80 (1997) 231–238.
[8] H. Narushima, N. Misheva, On a role of the MPR-poset of most-parsimonious reconstructions in phylogenetic analysis—a combinatorial optimization problem in phylogeny, in: W.Y.C. Chen, D.Z. Du, D.F. Hsu, H.Y. Hap (Eds.), Proceedings of the International Symposium on Combinatorics and Applications, Vol. 28–30, June 1996, Tianjin, P.R. China, pp. 306–313.
[9] D.F. Robinson, Extending a function on a graph, Discrete Math. 6 (1973) 89–99.
[10] D.L. Swofford, W.P. Maddison, Reconstructing ancestral character states under Wagner parsimony, Math. Biosci. 87 (1987) 199–229.
[11] D.L. Swofford, W.P. Maddison, Parsimony, character-state reconstructions, and evolutionary inferences, in: R.L. Mayden (Ed.), Systematics, Historical Ecology, and North American Freshwater Fishes, Stanford University Press, California, 1992, pp. 186–223.